Research Journal of Pharmaceutical, Biological and Chemical Sciences, 2015, vol.6, N6, pages 1781-1786

Comparative analysis of mice acetylcholinesterases by functional amino acid residues and molecular screening

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Abstract

In this paper, we have measured the distances between the reference amino acid residues of the acetylcholinesterase (AChE) active site, which showed that the existing three-dimensional models either have no differences or have differences within the structures resolution. Using the method of molecular docking in AutoDock, we have carried out the AChE screening with ligands, which denied the result of a previous calculation and showed that the affinity energy of one ligand (e.g.: donepezil) with 23 structures of enzyme is in the range of -6 to -12 kcal/mol, which is impossible for those structures having no significant differences. Following this line of reasoning, we can make two different conclusions: firstly, the existing AChE models are similar in general, and the choice of a model for work shall be based on the structure resolution, and a variety of screening results are just special cases of interaction with the side radicals of amino acid residues; secondly, the amount of insignificant changes in the spatial structure of each protein contributes largely to the screening result.

Keywords

Acetylcholinesterase, Docking, Ligands, Molecular interactions, Molecular screening, Protein spatial structures